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Magnons at the Curie temperature

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ABSTRACT

Random phase approximations (RPA) have very successfully treated spin wave excitations in Heisenberg ferromagnets at low temperatures. The role played by these magnons at the order-disorder transition, however, has been a topic which has eluded RPA theories to date. In light of recent data (1), the idea of magnons at the Curie temperature and above has become more difficult to refute. This adds incentive to attempt to model interacting magnons at the Curie temperature. This work examines some attempts to formulate higher random phase approximations and discusses why they fail as they approach the transition temperature. A new interpretation of some work by Parmenter and the author (2) is presented. The nature of the approximations made in that work is discussed, and an attempt is made to eliminate incorrect contributions from the energetically disfavored paramagnetic state to the correct magnon renormalization. A solution is presented which has the proper low temperature behavior as demonstrated by Dyson (3) restored and the reentrant behavior eliminated. An examination of how close this model comes to behaving correctly is performed, and a comparison is made to some recent work by Parmenter (4).

PACS numbers: [illegible]

I INTRODUCTION

At low temperatures the Heisenberg model of a ferromagnet can easily be shown to exhibit magnons or spin waves. It seems quite plausible [illegible], that these magnons could be the mechanism behind the ferromagnetic phase transition. Dyson (3) in his detailed analysis of the low temperature behavior of the Heisenberg ferromagnet points out that the Holstein-Primakoff spin wave theory (5) exaggerates the apparent interaction between magnons. Kittel (6) suggested that magnons might be valid excitations for temperatures approaching the Curie temperature, T_c. When random-phase type approximations (RPA) were applied to the problem of magnons at non-zero temperature, the answers were gratifying up to about half of the Curie temperature or better, but were seen to fail or require unphysical assumptions near T_c. It was widely believed that this failure was due to the fact that at T_c the relative local magnetization σ vanishes, and the normalization factor on the magnon operator is proportional to $\sigma^{-1/2}$. This does not, however, imply that applied to the proper many body permanental wave function the magnon operator is ill defined. Early experimental evidence (7) suggested, and recent data clearly shows (1) that magnons exist right up to and even beyond Tc. These facts recently prompted Parmenter and the author (2) to attempt higher RPA approximations in order to get results valid closer to Tc. The results of these calculations were less than encouraging, but did provide insight into the true reason for the breakdown of RPA. In the following I present a new interpretation of those results.

2 THE MODEL

We take the simplest system of interest, an isotropic Heisenberg nearest neighbor exchange Hamiltonian on a simple cubic lattice,

$$H = -\frac{1}{2} J \sum_{ij}' \{S_i^+ S_j^- + S_i^z S_j^z\}. \qquad (1)$$

The prime on the summation indicates summing all indices but the last over the entire crystal and the last index over the six nearest neighbors. For further simplicity we choose $S = 1/2$. It is well known that at $T = 0$, the magnon defined by the operator

$$S_k^+ = N^{-1/2} (2\sigma)^{-1/2} \sum_i e^{i\vec{k}\cdot\vec{R}_i} S_i^+ \qquad (2)$$

has the energy spectrum

$$\begin{aligned} \hbar\omega_k &= \frac{J}{2} \sum_\ell' \{1 - e^{i\vec{k}\cdot\vec{R}_\ell}\}. \\ &\simeq \frac{J}{2} a^2 k^2 \end{aligned} \qquad (3)$$

where a is the lattice constant. The renormalization constant for finite temperature then is defined,

$$\sigma(T) = \hbar\omega_k(T)/\hbar\omega_k(T=0) \qquad (4)$$

3 REINTERPRETED HIGHER APPROXIMATIONS

In the previously mentioned paper, Parmenter and the author used a multi-commutator equation of motion scheme to calculate successive approximation for $\alpha(T)$. Defining the super operator

$$\mathbf{L}\, S_k^{\pm} \equiv [S_k^{\pm}, H],$$

the equation of motion becomes

$$\hbar\omega_k^{\pm}(T) S_k^{\pm} = ^{+} \mathbf{L}\, S_k^{\pm}.$$

Repeated application of the super operator $\mathbf{L}$ followed by a thermal averaging produces a higher order linearized equation

$$\hbar\omega_k(T) = 2\hbar\omega_k(0) \left\{(2\sigma J^n \gamma_0^n)^{-1} \langle [S_\ell^-, \mathbf{L}^n S_\ell^+]\rangle\right\}^{1/n}$$

or the implicit equation for $\alpha(T)$

$$\alpha^{(n)} = 2\left\{(2\sigma J^n \gamma_0^n)^{-1} \langle [S_\ell^-, \mathbf{L}^n S_\ell^+]\rangle\right\}^{1/n}$$

where n indicates the order of the approximation. The first order equation "dresses" the bare magnon so that the Hamiltonian propagates it back into itself. The higher order equations "dress" the magnon with already dressed interactions so the hamiltonian will multiply propagate it back into itself. Bowen (8) has pointed out that if C^+ is a single particle, the operators C^+, $\mathbf{L}\, C^+$, $\mathbf{L}^2 C^+$, etc. form a generalized Hilbert space. The nth order equation corresponds to approximating the infinite dimensional space by an n dimensional one. The approximations are all random phase in nature since pairs of operators are ultimately replaced by thermal averages.

Our first approximation turned out to be identical with that found by Michelene Bloch (9) using a variational principle on a truncated Holstein-Primakoff (5) Hamiltonian representation. This approximation suffered from the problem that was to persist to higher orders, the α versus T curve was reentrant. Worse still the relative local magnetization σ versus T was reentrant, implying a first order phase transition (Figure 1A). The implicit equation for this first approximation is

$$\alpha^{(1)} = 1-\rho,$$

$$\rho = \frac{1}{3N}\sum_k \sum_\ell{}' f_k \left[1-e^{i\vec{k}\cdot\vec{R}_\ell}\right] \qquad (5)$$

$$\text{and } f_k = \left[e^{\beta\hbar\omega_k} - 1\right]^{-1}, \; \beta = \frac{1}{k_B T}$$

The second and third approximations gave the clue to the true problem with simple RPA. The lower re-entrant branch of the α curve is an attempt of the RPA to include the energetically disfavored paramagnetic phase. The lower branch tries to follow the line along which $\sigma(T/\alpha) = 0$.

I recently reexamined the second and third order RPA approximations in hopes of isolating that portion appropriate along the upper branch. The implicit equations for these are

$$\alpha^{(2)} = 2(\sigma F_1/\gamma_0 + \sigma F_2/\gamma_0^2 + \sigma^2\gamma_0(\gamma_0-1)/\gamma_0^2 + 1/4\gamma_0)^{1/2} \tag{6}$$

and

$$\alpha^{(3)} = 2[4\sigma F_1 F_2/\gamma_0^3 + 2\sigma^2 F_2\ \gamma_0^2 + \sigma^2(\gamma_0-1)F_1/\gamma_0^2 + F_1/4\gamma_0^2 + \sigma^3(\gamma_0-1)(\gamma_0-2)/\gamma_0^3 + \sigma(3\gamma_0-2)/(4\gamma_0)^2]^{1/3} \tag{7}$$

where

$$F_1 = N^{-1}\sum_k f_k\gamma_k$$

$$F_2 = N^{-1}\sum_k f_k\gamma_k^2$$

f_k [illegible]

In order to extract the portion of these implicit equations valid on the upper branch I expand the radicals about $\sigma = 1/2$. Care must be taken in this expansion, however. Consider first expanding about $\sigma = 0$. There one would set $\sigma^2 = 0$. In the expansion about $\sigma = 1/2$ I then set $\sigma^2 = 1/4$. Failure to do this will yield a σ curve inconsistent with the Dyson low temperature results.

The reinterpreted second approximation then takes the form

$$\alpha^{(2)} = 1 - 3/2g + 1/2h \tag{8}$$

where

$$h \equiv 2N^{-1} \sum_k f_k \frac{(\gamma_o - \gamma_k)^2}{\gamma_o^2} \equiv 2 \left\langle \frac{(\gamma_o - \gamma_k)^2}{\gamma_o^2} \right\rangle$$

and g in the same notation is

$$g = 2N^{-1} \sum_k f_k \frac{(\gamma_o - \gamma_k)}{\gamma_o} \equiv 2 \left\langle \frac{(\gamma_o - \gamma_k)}{\gamma_o} \right\rangle .$$

Replacing sums by integrals and integrating over an infinite spherical zone I reduce eqn (8) to a form which may be solved numerically for α given T by Newton's method. The results are shown in Figure 1B. The magnetization is still reentrant, but just barely. This is clearly an improvement over the first approximation.

Going to the third approximation, I find

$$\alpha^{(3)} = 1 - g + 2/3h, \qquad (9)$$

and Figure 1C shows σ is no longer reentrant, but has a negative slope at Tc. It is also reassuring that the low temperature behavior is again given by

$$\alpha = 1 - g,$$

as several different approaches indicate it should be. There is some reason to believe that only odd order approximations are truly appropriate for single particle excitations. The even orders are probably more appropriate for collective excitations such as plasmons or phonons.

4 SECOND ORDER TRANSITION

Ideally one would have hoped to have found the slope of the magnetization to be negatively infinite rather than merely negative. Note, however, that the slope at Tc has gone from positive to negative as we went from 1st to 3rd approximations. To see how close this approximation comes to having a divergence in the slope of the magnetization, consider adding a multiplier to the third term in the implicit equation for α,

$$\alpha^{(3)} = 1 - g + 2/3\, ch.$$

It is simple to show that $c = .408$ will give the desired result. Figure 1D shows the results for this value of c. If you choose $c = .5$, the slope at Tc is nearly infinite and the α curve bears a striking resemblance to the data presented by Bohn, Zinn, Dorner, and Kollmar at the 1981 conference on Magnetism and Magnetic Materials (1), exhibiting magnons both below and above Tc. See Figure 1F. Parmenter (4) has suggested this as a fundamental requirement for the α renormalization curve. He allows α to depend on T only thru powers of the function g,

$$\alpha = 1 - g + C_2 g^2 + C_3 g^3 + C_4 g^4 .$$

He then requires

$$\left.\frac{\partial T(g)}{\partial g}\right|_{Tc} = \left.\frac{\partial^2 T(g)}{\partial g^2}\right|_{Tc} = 0 \quad \text{and} \quad \left.\frac{\partial^3 T(g)}{\partial g^3}\right|_{Tc} > 0.$$

Figure 1F shows the results from solving Parmenter's implicit α curve numerically.

While this paper does not demonstrate a first principles RPA theory which correctly predicts thermodynamic behavior at the order-disorder transition, I believe it has shown that RPA theories are not as far in error as is commonly believed. After the more than twenty years that people have worked on this problem, I believe we are beginning to see where the real difficulties with simple RPA theories lie. The keys to understanding this problem are first the existence of magnons at and above Tc and second the complications of the energetically disfavored paramagnetic state below Tc.

REFERENCES

1. H.G. Bohn, W. Zinn, B. Dorner, A. Kollmar, J. Appl. Phys. 52, 2228 (1981)

2. D.A. Poling and R.H. Parmenter, Phys. Rev. B 16, 3240, (1977)

3. F.J. Dyson, Phys. Rev. 102, 1217 (1956)

4. R.H. Parmenter (unpublished)

5. T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940)

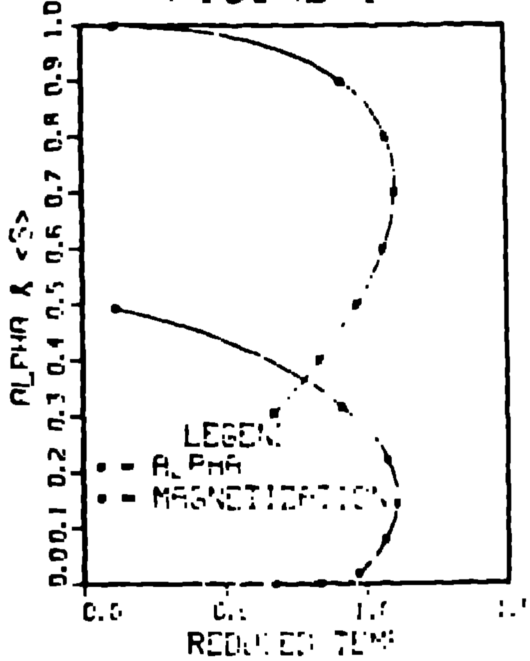
6. C. Kittel, International Conference on Magnetic Relaxation, Eindhoven, July 1962 (unpublished)

7. B. Jacrot and D. Cribier, J. Phys. Radium 23, 494 (1962)

8. S.P. Bowen, J. Math. Phys. 16, 620 (1975)

9. M. Bloch, J. Appl. Phys. 34, 1151 (1963)

FIGURE 1



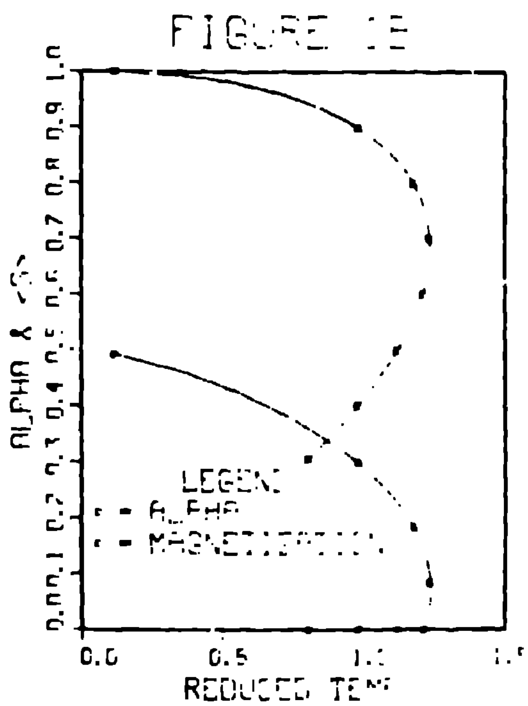


FIGURE 1B
LEGEND
ALPHA
MAGNETIZATION
REDUCED TEMP
0.0
0.5
1.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9

FIGURE 11

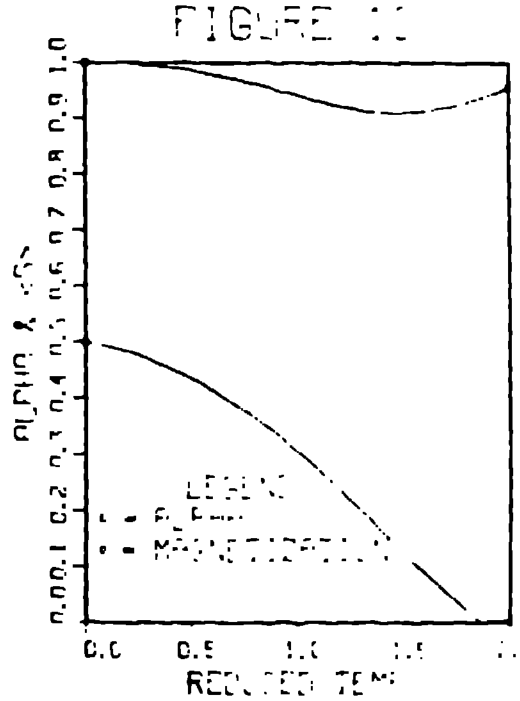
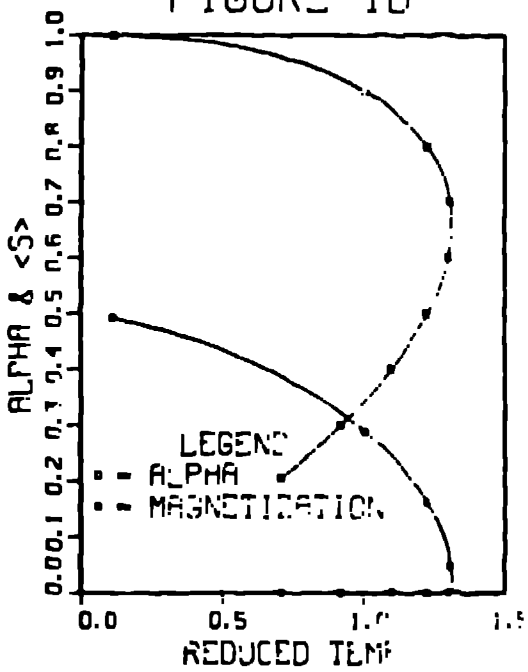

1.0
0.9
0.8
0.7
0.6
0.4
0.2
0.1
0.0
0.5
1.0
LEGEND
MAGNETIZATION
REDUCED TEMP

FIGURE 1D



ALPHA & <S>
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
LEGEND
ALPHA
MAGNETIZATION
0.0
0.5
1.0
1.5
REDUCED TEMP

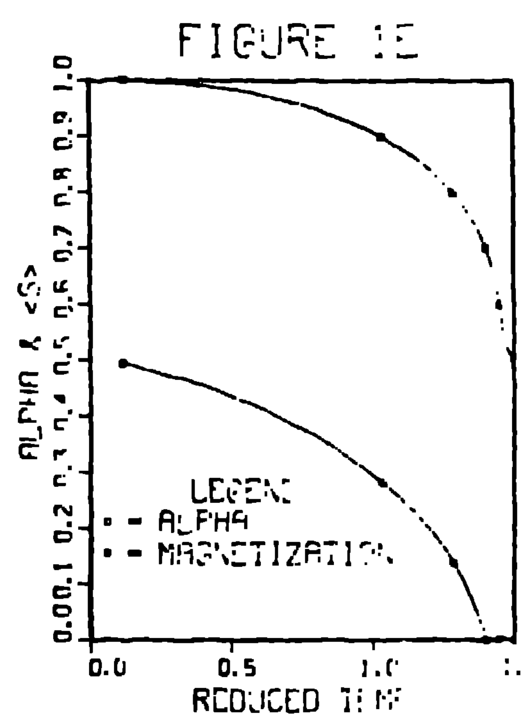


FIGURE 1E
ALPHA & <S>
0.0
0.5
1.0
REDUCED TEMP
LEGEND
ALPHA
MAGNETIZATION